

# New UCODE\_2005 Input Blocks for Defining Parameters Applicable Only to Prediction Conditions

## *Introduction*

### **Problem**

Simulation models of natural and engineered processes commonly are developed and calibrated for the purpose of predicting values, for example, at a future time or under different boundary conditions. The model used for simulating the predictions might require parameters that are not applicable to the calibration conditions. For example, a ground-water flow model might be calibrated for long-term steady-state conditions, and used to predict transient drawdown under future pumping. In this case, the predictive model requires storage parameters not applicable to the calibrated model.

UCODE\_2005 version 1.007 (and earlier versions) requires that an identical set of parameters be defined for a prediction run (Mode = Prediction) and for the sensitivity (Mode = Sensitivity-Analysis) or calibration (Mode = Parameter-Estimation) run that precedes the prediction run. Therefore, if there are parameters applicable only to the prediction simulation, then these parameters must still be defined for the sensitivity or calibration run, even though the sensitivities of the observations to these parameters equal zero. Defining these prediction-only parameters in the sensitivity or calibration run can be cumbersome.

### **Purpose and Scope**

To streamline the definition of parameters applicable only to prediction simulations, new capabilities have been added to UCODE\_2005 version 1.009<sup>1</sup> to allow defining parameters for prediction runs in the situation where these parameters are not defined for the preceding sensitivity or calibration run. Prior information on these parameters also can be defined.

These capabilities can be used to more easily produce scaled and unscaled prediction sensitivities with respect to parameters that are applicable only to the prediction run, compared to producing this output in previous versions of UCODE\_2005. The capabilities also can be used to define prior information on these parameters, which represents their uncertainty. Through the use of data-exchange files, the sensitivities and uncertainty can then be accounted for in prediction uncertainty measures. Such measures include the linear intervals calculated by the computer code LINEAR\_UNCERTAINTY (Poeter and others, 2005), the nonlinear intervals calculated by UCODE\_2005, and the statistics calculated by OPR-PPR (Tonkin and others, 2007) which can be used to identify data likely to reduce prediction uncertainty.

This document describes the new UCODE\_2005 capability of defining parameters and prior information only for prediction runs, and describes the associated model input and output.

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<sup>1</sup> version 1.008 was a temporary internal version that was not released

### ***New input blocks***

Five new input blocks have been defined to accommodate the new UCODE\_2005 capabilities related to parameters that are only applicable to prediction conditions. The blocklabels for the new input blocks are shown in bold italic type in table 1, in the order in which the new input blocks must appear in the main UCODE\_2005 input file relative to other input blocks. The name of each new input block builds on the name of an existing input block, by appending the phrase *\_For\_Prediction* to the name of the existing block, as shown in table 1.

Table 1. Blocklabels of the main input file for UCODE\_2005, including blocklabels for the new input blocks described in this report. Modified from Poeter and others (2005, Table 4, p. 43).

[Bold type and grey shading identify required input blocks; the other input blocks are optional. Bold italic type identifies new optional input blocks described in this report. See Poeter and others (2005, Table 4) for footnotes.]

Purpose	Blocklabel	Default column order <sup>2</sup>
Define UCODE_2005 operation	Options	No
	Merge_Files	No
	UCODE_Control_Data	No
	Reg_GN_Controls	No
	Reg_GN_NonLinInt	No
	<b>Model_Command_Lines</b>	No
Define parameters	Parameter_Groups	No
	<i>Parameter_Groups_For_Prediction</i>	No
	<b>Parameter_Data</b>	Yes
	<i>Parameter_Data_For_Prediction</i>	Yes
	Parameter_Values	Yes
	Derived_Parameters	Yes
	<i>Derived_Parameters_For_Prediction</i>	Yes
Define observations	Observation_Groups	No
	<b>Observation_Data</b>	Yes
	Derived_Observations	Yes
Define predictions	Prediction_Groups	No
	<b>Prediction_Data</b>	Yes
	Derived_Predictions	Yes
Define prior information	Prior_Information_Groups	No
	<i>Prior_Information_Groups_For_Prediction</i>	No
	Linear_Prior_Information	Yes
	<i>Linear_Prior_Information_For_Prediction</i>	Yes
Define variance-covariance matrices to weight groups of observations or prior information with correlated errors.	Matrix_Files	No
Interact with process-model input and output files.	<b>Model_Input_Files</b>	Yes
	<b>Model_Output_Files</b>	Yes
Run process model(s) using multiple processors	Parallel_Control	No
	Parallel_Runners	Yes

## **Input to Define Parameters Applicable Only to Prediction Conditions and to Define Prior Information on these Parameters**

For each of the new input blocks, the keywords are exactly the same as those for the existing input block that has a similar name (without `_For_Prediction` appended).

### ***Parameter\_Groups\_For\_Prediction (optional)***

Use this input block to assign data that apply to all or many of the parameters defined only for the predictions. When quantities specified in the `Parameter_Groups_For_Prediction` input block are repeated in the `Parameter_Data_For_Prediction` block, the data specified in the `Parameter_Data_For_Prediction` block are used. Keywords in this input block are described in Poeter and others (2005, p. 68).

### ***Parameter\_Data\_For\_Prediction (optional)***

Use this input block to assign data to individual parameters defined only for the predictions. Information about use of this block, and keywords in this input block, are described in Poeter and others (2005, p. 69-72).

### ***Derived\_Parameters\_For\_Prediction (optional)***

Use this input block to define parameters derived from parameters defined in the `Parameter_Data_For_Prediction` input block. Keywords in this input block are described in Poeter and others (2005, p. 76).

### ***Prior\_Information\_Groups\_For\_Prediction (optional)***

Use this input block to assign data that apply to many or all of the items of prior information defined in the `Linear_Prior_Information_For_Prediction` input block. When quantities specified in the `Prior_Information_Groups_For_Prediction` input block are repeated in the `Linear_Prior_Information_For_Prediction` block, the data specified in the `Linear_Prior_Information_For_Prediction` block are used. Keywords in this input block are described in Poeter and others (2005, p. 94).

### ***Linear\_Prior\_Information\_For\_Prediction (required if Parameter\_Data\_For\_Prediction input block exists)***

Use this input block to assign data related to individual items of prior information on parameters defined only for prediction conditions. Information about use of this block, and keywords in this input block, are described in Poeter and others (2005, p. 95-96).

The `Linear_Prior_Information_For_Prediction` input block is required if the `Parameter_Data_For_Prediction` input block exists, for the following reason. Parameters typically will be defined in the `Parameter_Data_For_Prediction` input block so that their sensitivities and uncertainty can be included in the calculation of measures of prediction uncertainty by, for example, the codes `LINEAR_UNCERTAINTY` (Poeter and others, 2005) and `OPR-PPR` (Tonkin and others, 2007). Because these parameters are not defined for the calibrated model, definition of prior information on these parameters is the only mechanism for including their uncertainty in the parameter variance-covariance matrix. This matrix is the means by which parameter uncertainty is included in measures of prediction uncertainty. The required definition of prior information on these parameters is accomplished using the

Linear\_Prior\_Information\_For\_Prediction block and, optionally, the Prior\_Information\_Groups\_For\_Prediction block.

## **Output Files Related to Parameters Defined Only for Prediction Conditions**

### **Changes to Existing Output Files**

Data-exchange file *\_dmp* includes a second line with the label "NUMBER OF PARAMETERS FOR PREDICTIVE EVALUATION = ", which reports the total number of parameters defined for prediction conditions.

Data-exchange files *\_sppp*, *\_sppr*, *\_spsp*, *\_spsr*, and *\_spu* include sensitivities for parameters defined only for prediction conditions.

Data-exchange file *\_pv* has the same appearance, but calculated prediction variances include the effects of prediction sensitivities for parameters defined only for prediction conditions, and of the uncertainty in these parameters as expressed through the definition of their prior information.

### **New Output Files**

Data-exchange files *\_suprip* and *\_wtprip* are produced when parameters are defined in the Parameter\_Data\_For\_Prediction input block and, as required when this input block exists, prior information on these parameters is defined in the Linear\_Prior\_Information\_For\_Prediction block and, optionally, the Prior\_Information\_Groups\_For\_Prediction block.

File *\_suprip* has the same contents as file *\_supri* (Poeter and others, 2005, table 18, p. 153), except that PRIOR NAME is the name of a prior information equation defined in the Linear\_Prior\_Information\_For\_Prediction, and Param-Name1, Param-Name2, and so on, are names of parameters defined in the Parameter\_Data\_For\_Prediction.

File *\_wtprip* has the same contents as file *\_wtpri* (Poeter and others, 2005, table 17, p. 152), except that the number of rows equals the number of prior information equations defined in the Linear\_Prior\_Information\_For\_Prediction input block.

### **Example**

Example *ex1b* in the distribution for UCODE\_2005 version 1.009 uses the new capabilities described in this document. In the distribution, this example is in the folder *ucode\_2005\_1.009\test-win\ex1b*. In this example, a transient model is calibrated using head, drawdown, and flow observations, and is then used to predict an advective transport path. The prediction requires that an effective porosity parameter be defined; this parameter is not applicable to the calibration run. The input file for the prediction run is named *15.in*. Figure 1 lists input blocks in *15.in* that pertain to the definition of parameters, predictions, and prior information. The input blocks that are described in this document are shown in bold type.

```

# -----
# PARAMETER INFORMATION
# -----

BEGIN PARAMETER_GROUPS KEYWORDS
  GroupName = MyPars adjustable=yes TOLPAR=.01 SenMethod=2
  MaxChange=2.0
END PARAMETER_GROUPS

BEGIN PARAMETER_GROUPS_FOR_PREDICTION KEYWORDS
  GroupName=porgroup adjustable=yes TOLPAR=.01 SenMethod=2
  MaxChange=2.0
END PARAMETER_GROUPS_FOR_PREDICTION

BEGIN PARAMETER_DATA FILES
  ..\exlb-files\tr.params
END PARAMETER_DATA

BEGIN PARAMETER_DATA_FOR_PREDICTION TABLE
#   1       2       3       4       5       6       7       8       9
nrow=1 ncol=9 columnlabels
paramname STARTVALUE lowervalue uppvvalue scalepval perturbamt transform TOLPAR groupname
  POR_1&2 0.33 0.27 0.39 0.33 0.01D0 no 0.01
porgroup
END PARAMETER_DATA_FOR_PREDICTION

# -----
# PREDICTION INFORMATION
# -----

BEGIN PREDICTION_GROUPS FILES
  ..\exlb-files\groups.pred
END PREDICTION_GROUPS

BEGIN PREDICTION_DATA FILES
  ..\exlb-files\adv.pred
END PREDICTION_DATA

# -----
# PRIOR INFORMATION
# -----

BEGIN PRIOR_INFORMATION_GROUPS_FOR_PREDICTION KEYWORDS
GroupName=prior
PlotSymbol=4
UseFlag=yes
END PRIOR_INFORMATION_GROUPS_FOR_PREDICTION

BEGIN LINEAR_PRIOR_INFORMATION_FOR_PREDICTION KEYWORDS
PriorName=PrPorosity
Equation=POR_1&2
PriorInfoValue=0.33
Statistic=0.03
StatFlag=SD
GroupName=prior
END LINEAR_PRIOR_INFORMATION_FOR_PREDICTION

```

Figure 1. Part of file *15.in* included in the distribution of UCODE\_2005 version 1.009, showing input blocks for the definition of an effective porosity parameter that is only applicable to the prediction run, and of prior information on this parameter. Input blocks described in this document are shown in bold type.

## ***References***

- Poeter, E.P., Hill, M.C., and Banta, E.B., 2005, UCODE\_2005 and six other computer codes for universal sensitivity analysis, calibration, and uncertainty evaluation: U.S. Geological Survey Techniques and Methods, book 6, sec. A, chap. 11, 283 p.
- Tonkin, M.J., Tiedeman, C.R., Ely, D.M., and Hill, M.C., 2007, OPR-PPR, A computer program for assessing data importance to model predictions using linear statistics: U.S. Geological Survey Techniques and Methods, book 6, sec. E, chap. 2, 113 p.